STN Search - CASREACT 10/785,627 Strategy

03/15/2006

6 7 8 9 16 17 18 19 25 26 27 28 29 30

ring nodes :

1 2 3 4 5 11 12 13 14 15

chain bonds :

2-26 4-6 4-7 5-29 5-30 6-8 6-9 11-25 13-16 13-17 14-27 14-28 16-18 16-19

ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

1-2 1-5 2-3 2-26 3-4 4-5 4-6 4-7 5-29 5-30 6-8 6-9 11-12 11-15 11-25

12-13 13-14 13-16 13-17 14-15 14-27 14-28 16-18 16-19

isolated ring systems :

containing 1 : 11 :

G1:0,S

G2:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS

25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

containing 11

node mappings:

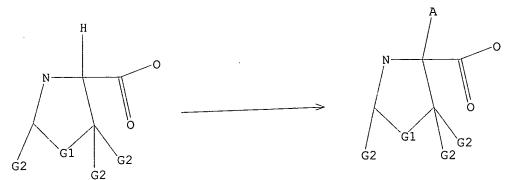
2:11 3:12 4:13 5:14 6:16 6:16

L1STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 0, S

G2 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 22:23:30 FILE 'CASREACT'

SCREENING COMPLETE - 45706 REACTIONS TO VERIFY FROM

2850 DOCUMENTS

100.0% DONE 45706 VERIFIED

75 HIT RXNS

17 DOCS

SEARCH TIME: 00.00.01

17 SEA SSS FUL L1 (75 REACTIONS)

=> d ibib abs hit 1-17